Electronic Supplementary Information Fischer *et al.*

Table of contents

NMR spectra

^{1}H-NMR of compound **2b** (MeOH-d_4; recorded after H/D exchange)	Figure S1.
^{13}C-NMR of compound **2b** (MeOH-d_4; recorded after H/D exchange)	Figure S2.

MS spectra

HRMS (ESI) of compound **2b**	Figure S3.
MS (MALDI-TOF) of compound **12**	Figure S4.
MS (MALDI-TOF) of compound [Re(CO)$_3$(**12**)]	Figure S5.
MS (MALDI-TOF) of compound **13**	Figure S6.
MS (MALDI-TOF) of compound [Re(CO)$_3$(**13**)]	Figure S7.
MS (MALDI-TOF) of compound **14**	Figure S8.
MS (MALDI-TOF) of compound [Re(CO)$_3$(**14**)]	Figure S9.
MS (MALDI-TOF) of compound **15**	Figure S10.
MS (MALDI-TOF) of compound [Re(CO)$_3$(**15**)]	Figure S11.

HPLC chromatograms

HPLC chromatograms of compound **14**, [Re(CO)$_3$(**14**)], and [^{99m}Tc(CO)$_3$(**14**)]	Figure S12.
HPLC chromatograms of compound **15**, [Re(CO)$_3$(**15**)], and [^{99m}Tc(CO)$_3$(**15**)]	Figure S13.

Figure S1. [1]H-NMR of compound **2b** (MeOH-d_4; recorded after H/D exchange).

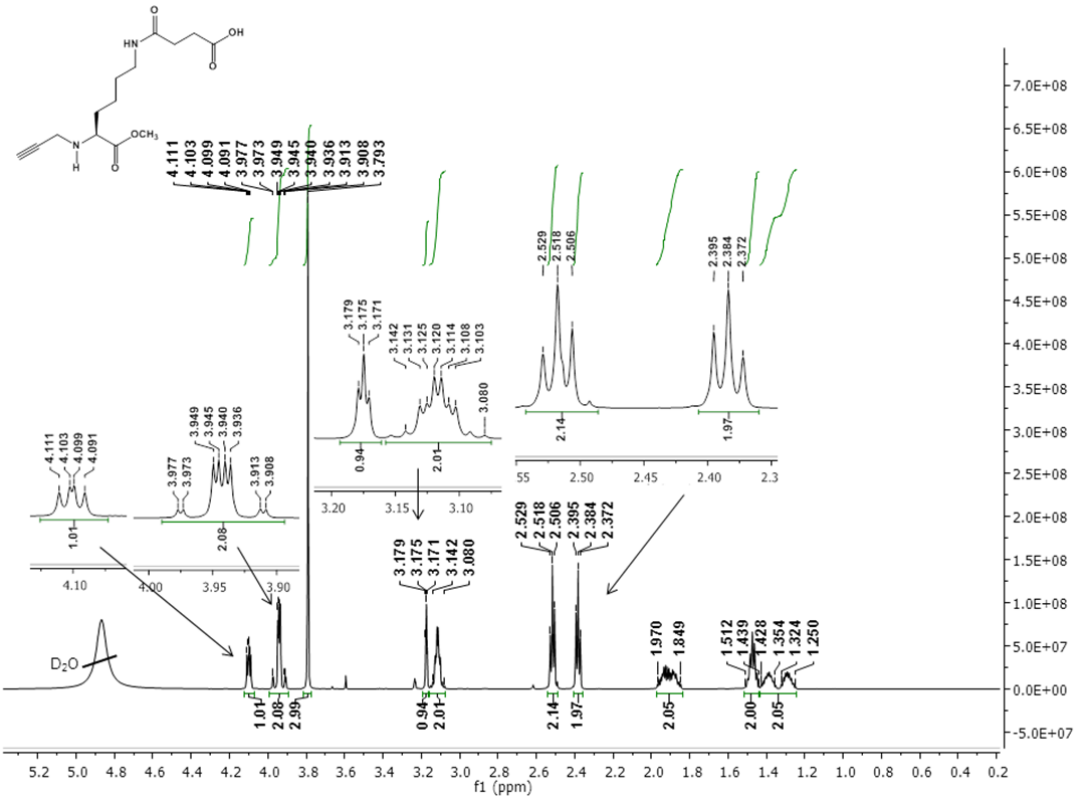


Figure S2. [13]C-NMR of compound **2b** (MeOH-d_4; recorded after H/D exchange).

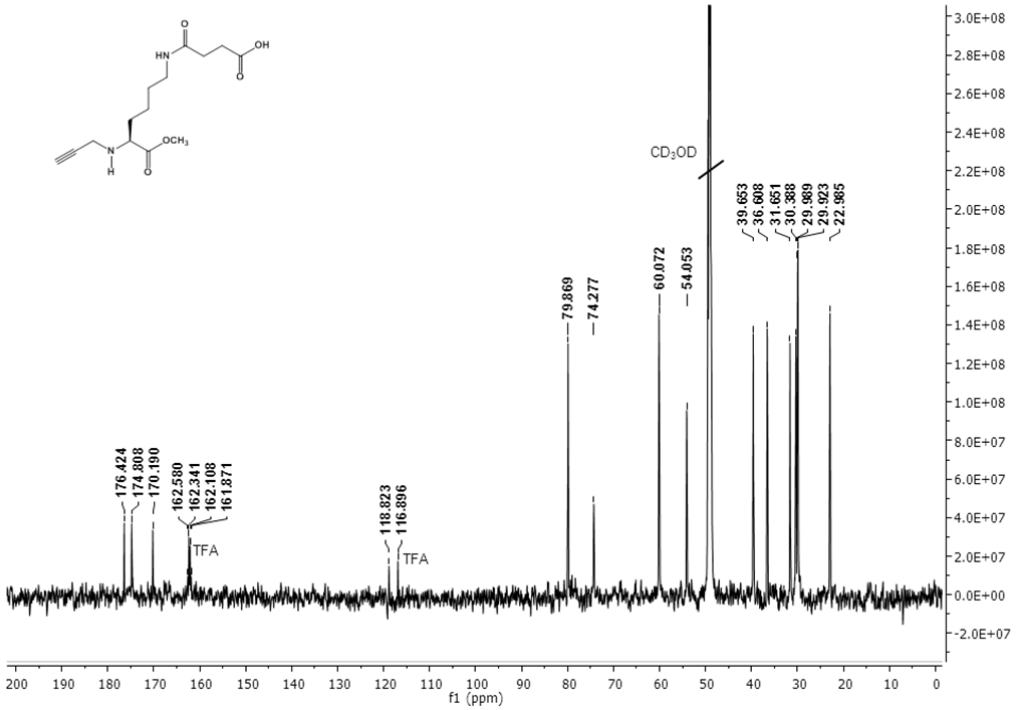


Figure S3. HRMS (ESI) of compound **2b**.

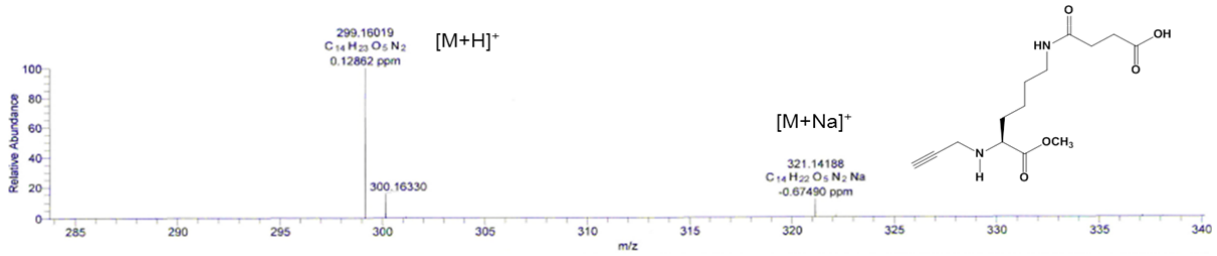


Figure S4. MS (MALDI-TOF) of compound **12**.

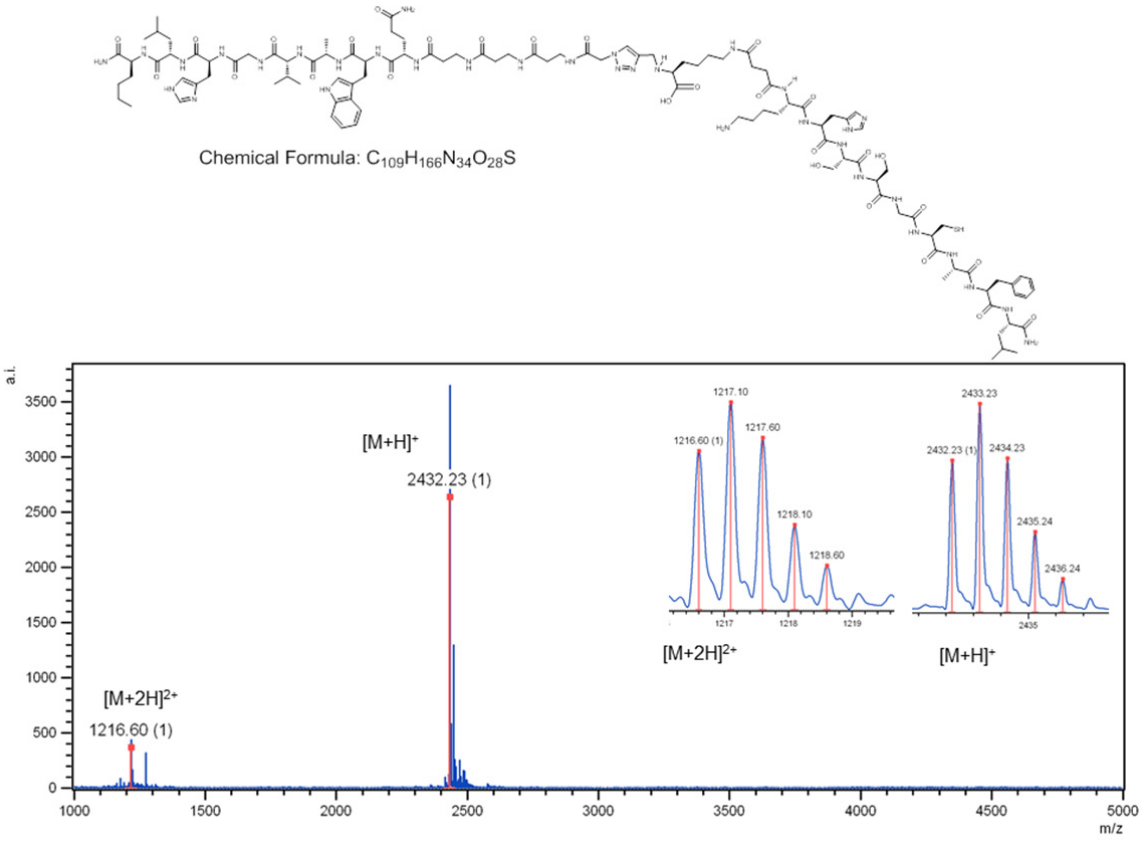


Figure S5. MS (MALDI-TOF) of compound [$Re(CO)_3$(**12**)].

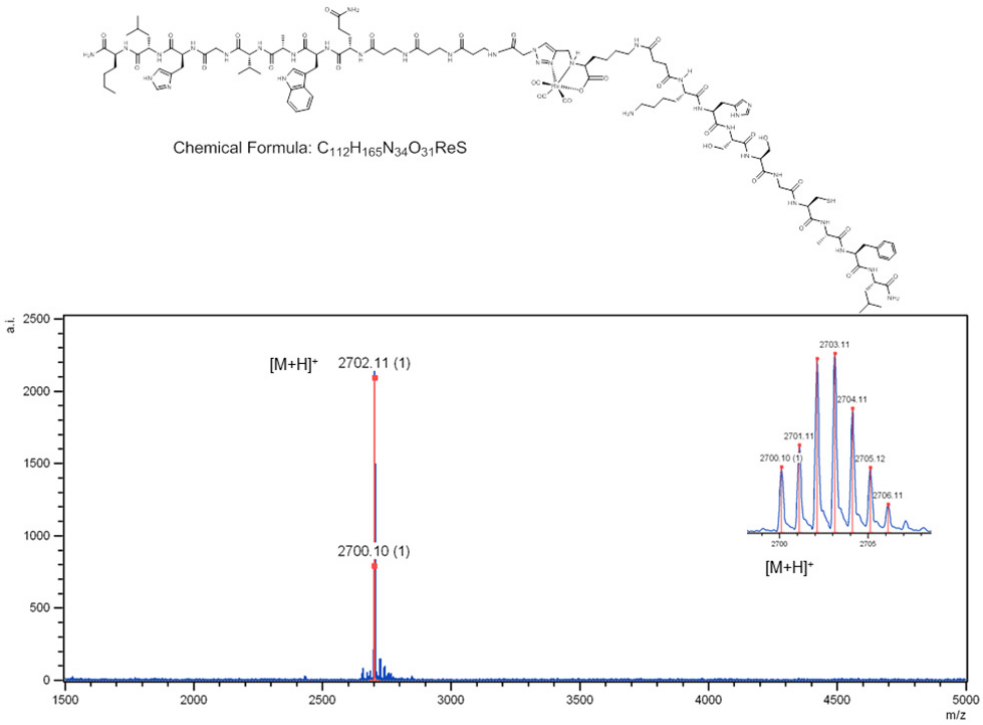


Figure S6. MS (MALDI-TOF) of compound **13**.

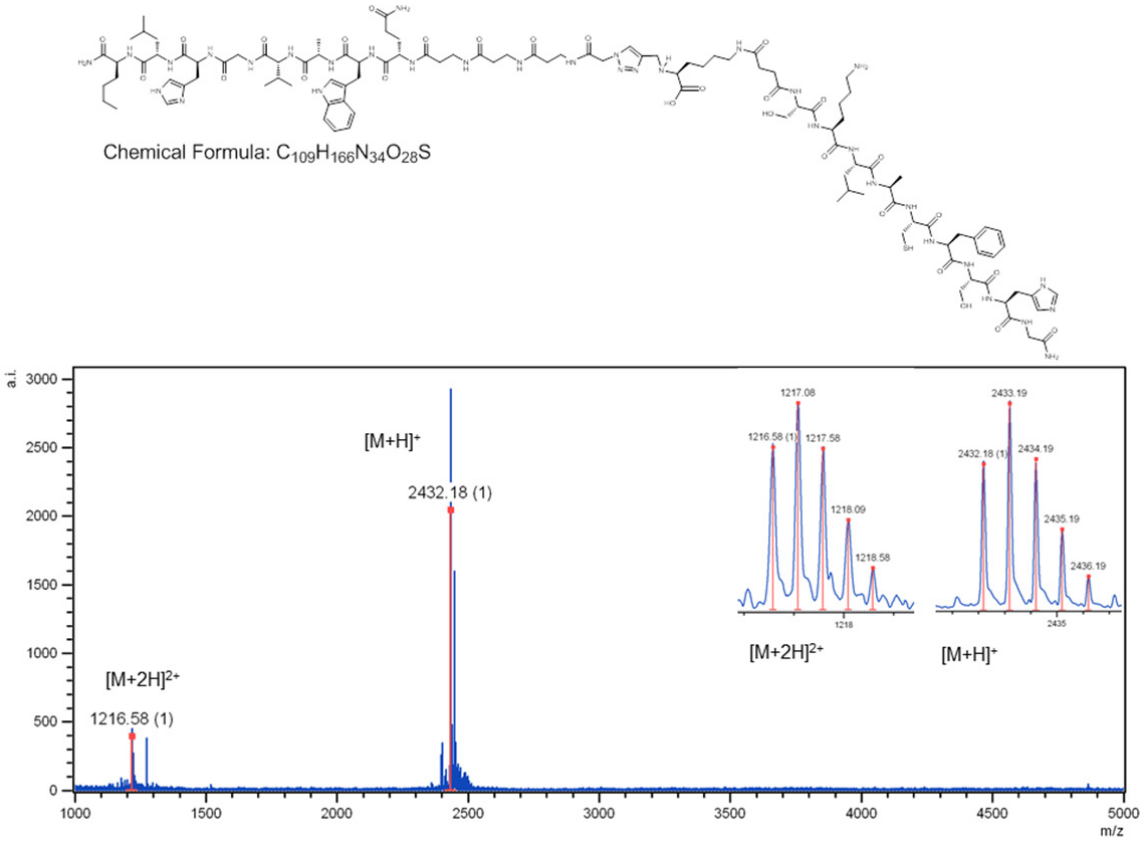


Figure S7. MS (MALDI-TOF) of compound [$Re(CO)_3$(**13**)].

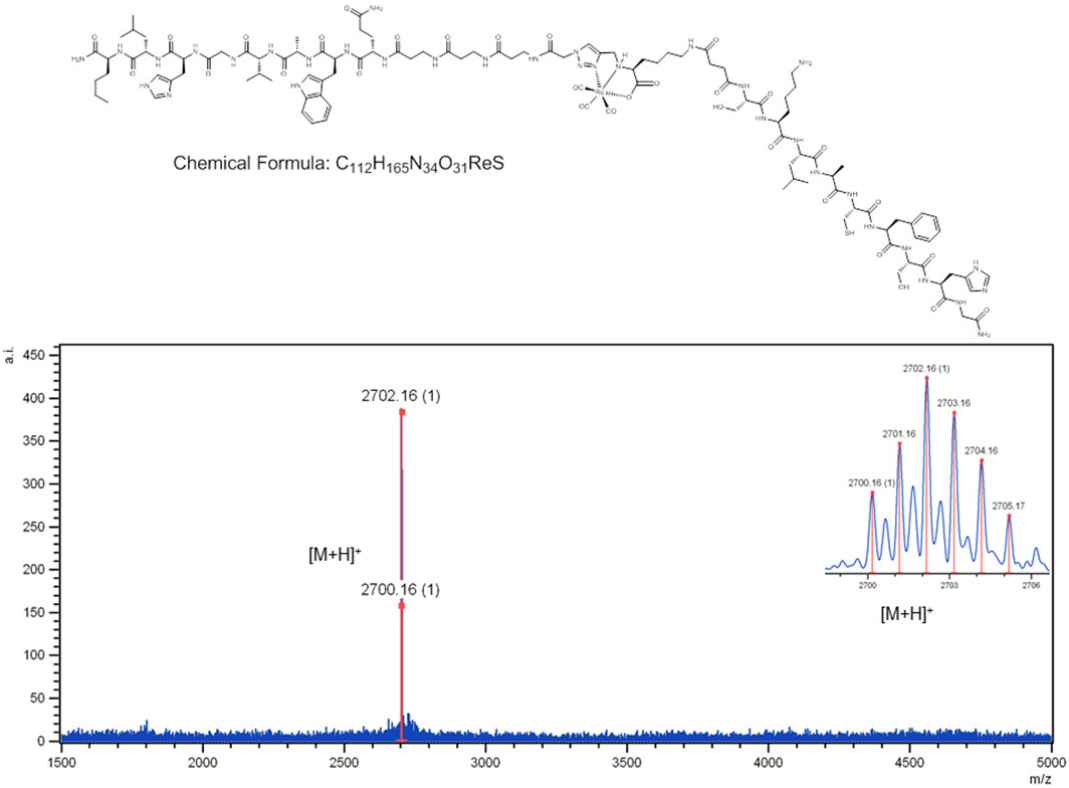


Figure S8. MS (MALDI-TOF) of compound **14**.

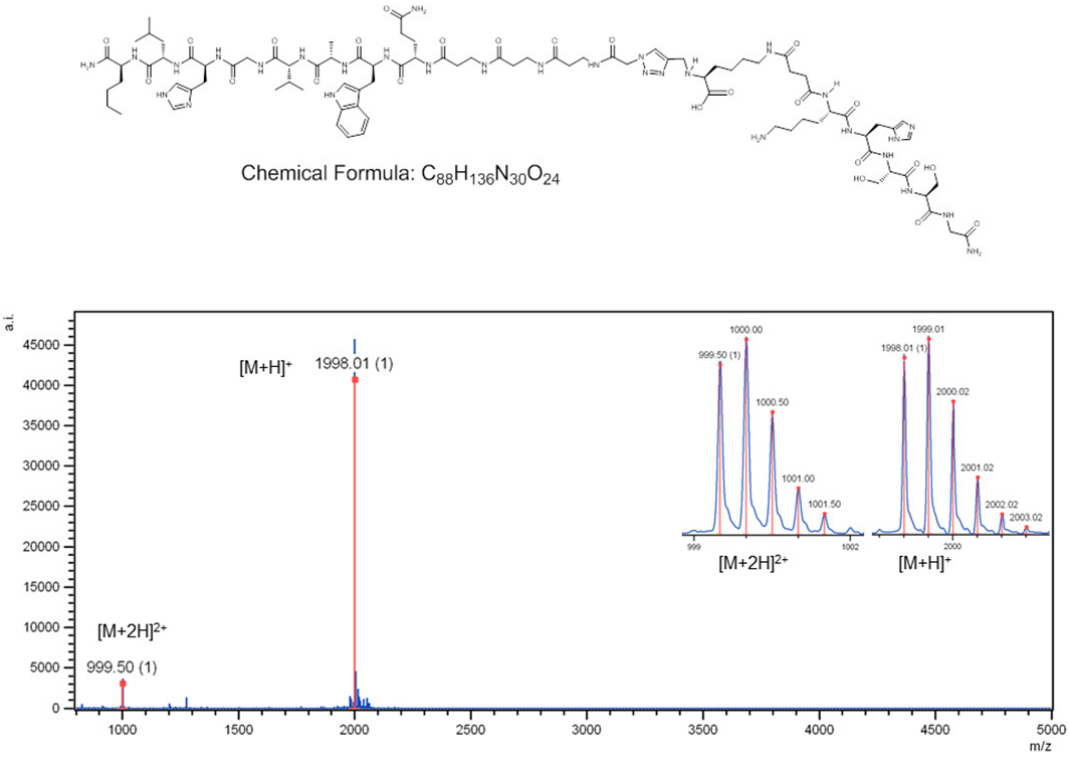
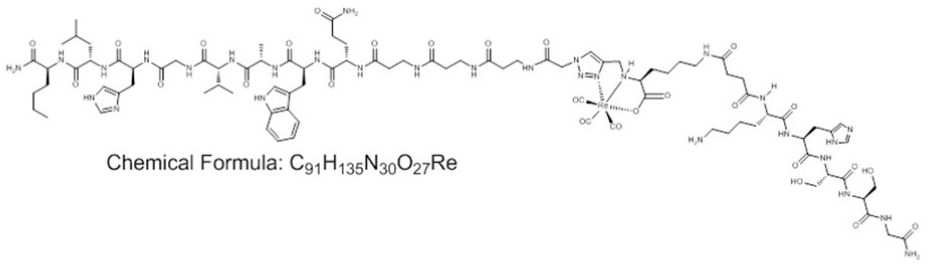


Figure S9. MS (MALDI-TOF) of compound [$Re(CO)_3$(**14**)].



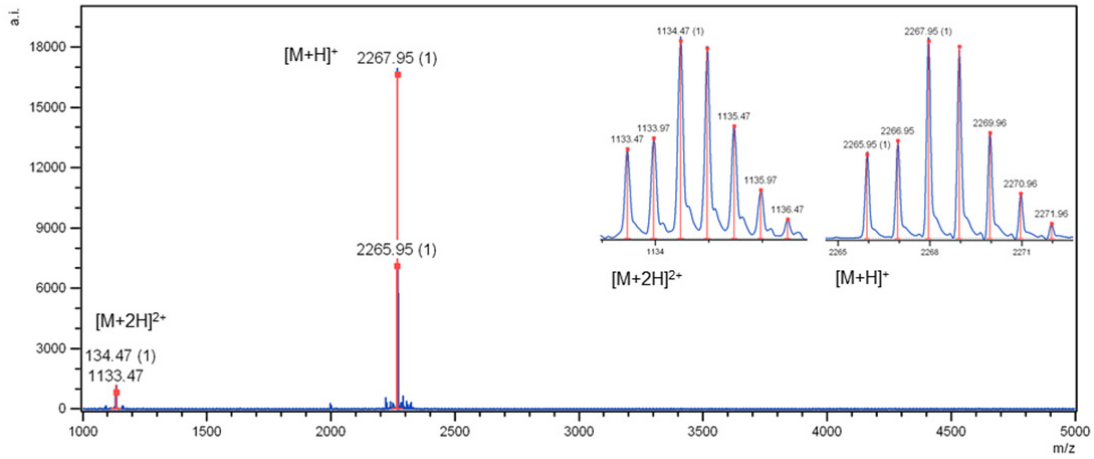
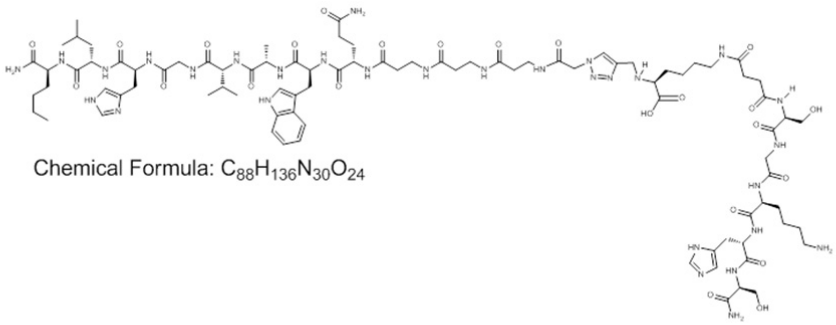


Figure S10. MS (MALDI-TOF) of compound **15.**



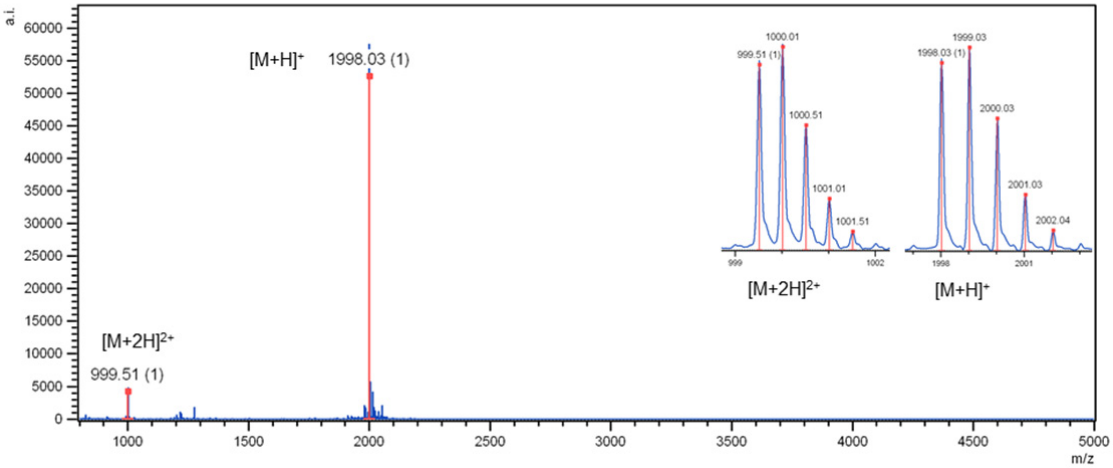


Figure S11. MS (MALDI-TOF) of compound [$Re(CO)_3$(**15**)].

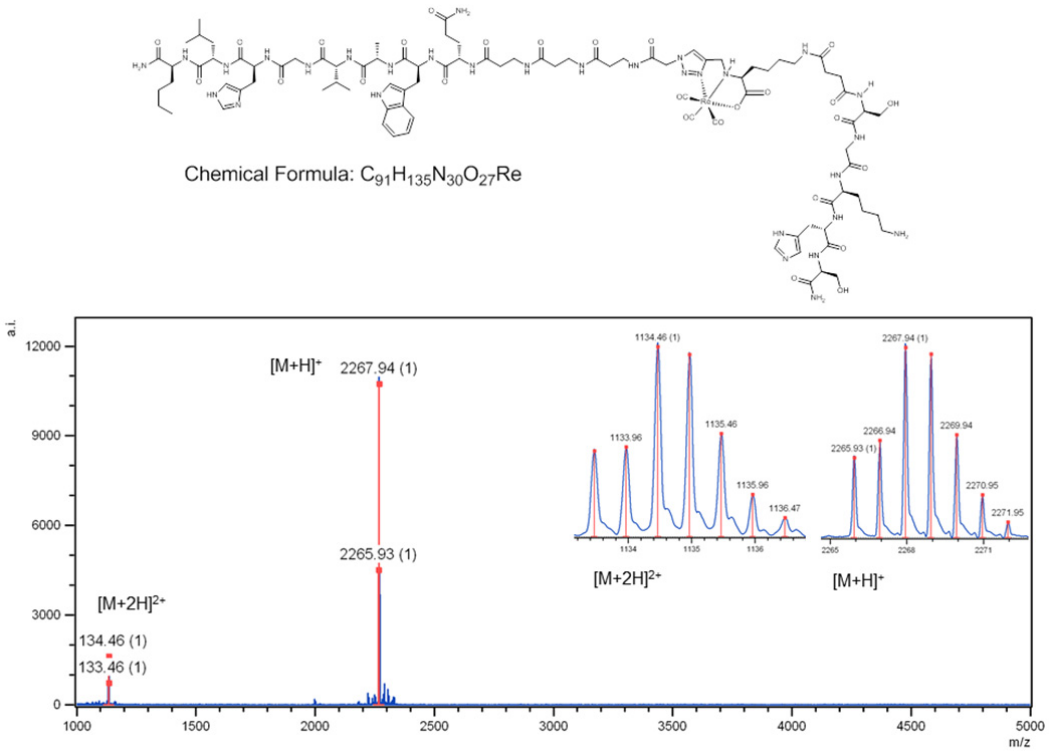
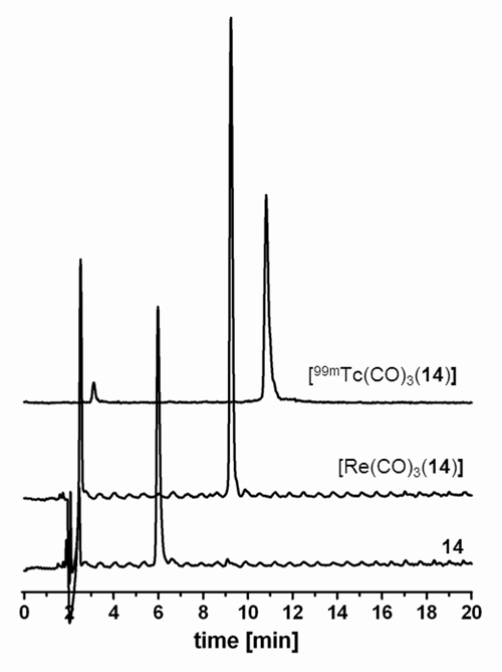
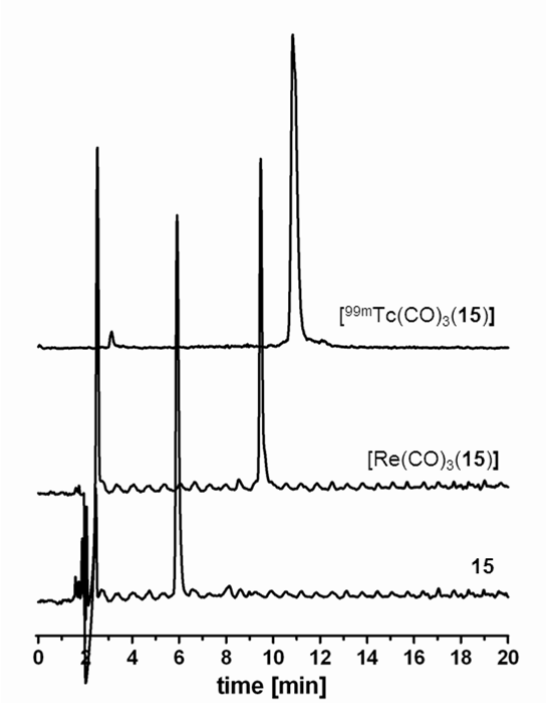


Figure S12. HPLC chromatograms of compound **14**, [$Re(CO)_3$(**14**)], and [$^{99m}Tc(CO)_3$(**14**)].



HPLC chromatograms of peptide **14** (UV-race, 214 nm), the corresponding metal conjugates [$Re(CO)_3$(**14**)] (UV-trace, 214 nm), and [$^{99m}Tc(CO)_3$(**14**)] (γ-trace); column A and a linear gradient from 80% A to 50 % A in 20 min with a flow rate of 1.5 mL/min. The small difference of retention times between [$Re(CO)_3$(**14**)] and [$^{99m}Tc(CO)_3$(**14**)] is due to the serial arrangement of the UV- and γ-detectors.

Figure S13. HPLC chromatograms of compound **15**, [Re(CO)$_3$(**15**)], and [^{99m}Tc(CO)$_3$(**15**)].



HPLC chromatograms of peptide **15** (UV-race, 214 nm), the corresponding metal conjugates [Re(CO)$_3$(**15**)] (UV-trace, 214 nm), and [^{99m}Tc(CO)$_3$(**15**)] (γ-trace); column A and a linear gradient from 80% A to 50 % A in 20 min with a flow rate of 1.5 mL/min. The small difference of retention times between [Re(CO)$_3$(**15**)] and [^{99m}Tc(CO)$_3$(**15**)] is due to the serial arrangement of the UV- and γ-detectors.